Dephosphorylation reactions with deferoxamine, a potential chemical nuclease

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Electronic Supporting Information

1. Kinetic data

Table S.1. Rate constants as a function of pH for the reaction of **DFO** with **BDNPP** at 25.0°C in water, μ = 1.0 M (KCl).

pH	**10^2 k_2, $M^{-1}s^{-1}$**
7.07	0.0145
7.47	0.0183
8.01	0.0576
8.51	0.185
9.04	0.627
9.30	1.22
9.52	1.69
9.70	2.10
9.80	2.45
9.98	2.75
10.2	3.08
10.3	3.39
10.5	3.61
10.6	3.68
10.9	3.82
11.1	3.89
11.3	3.89
11.5	3.90

2. ESI-MS spectrometry

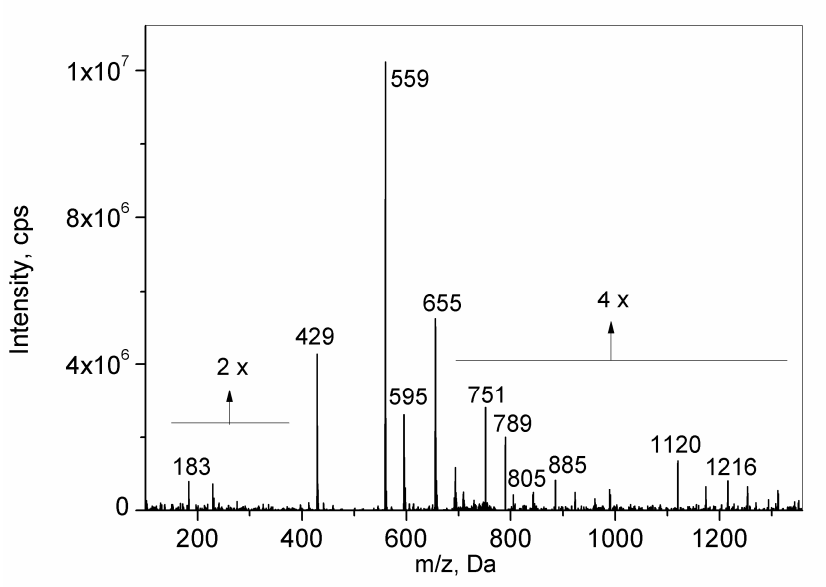
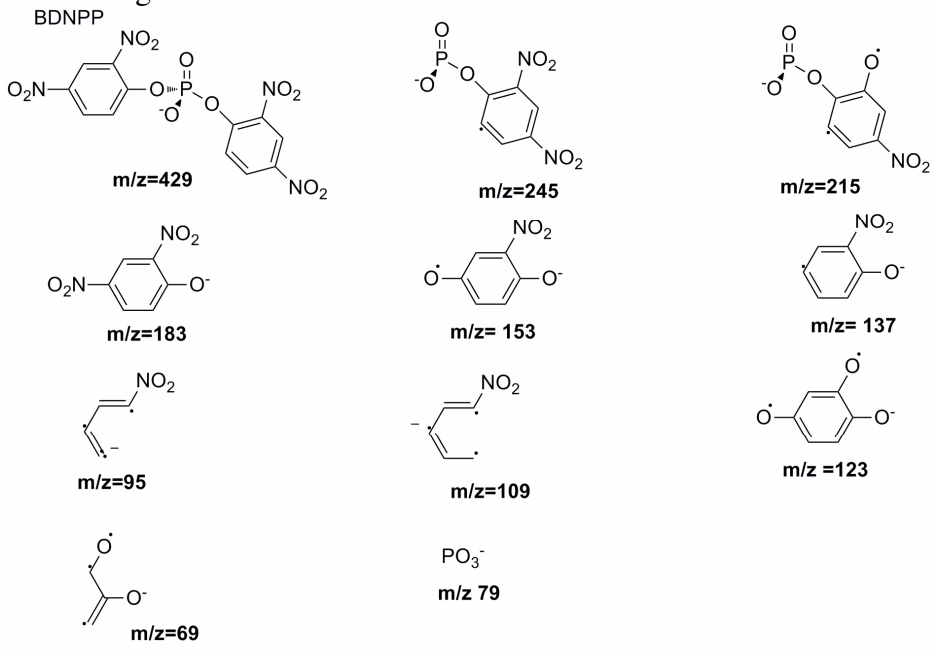


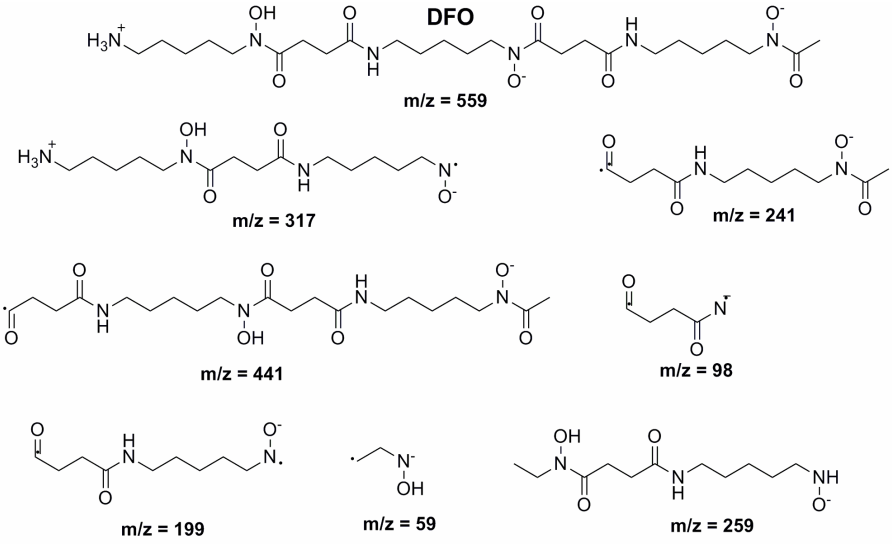
Figure S2. ESI-MS (-) after 30 min of reaction of **BDNPP** with **DFO** in aqueous solution at pH 10 and 25°C.

Scheme S3. ESI-MS/MS fragment assignments for **BDNPP** of m/z 429, **DFO** of m/z 559 and the proposed phosphorylated intermediates of m/z 805 and m/z 885.

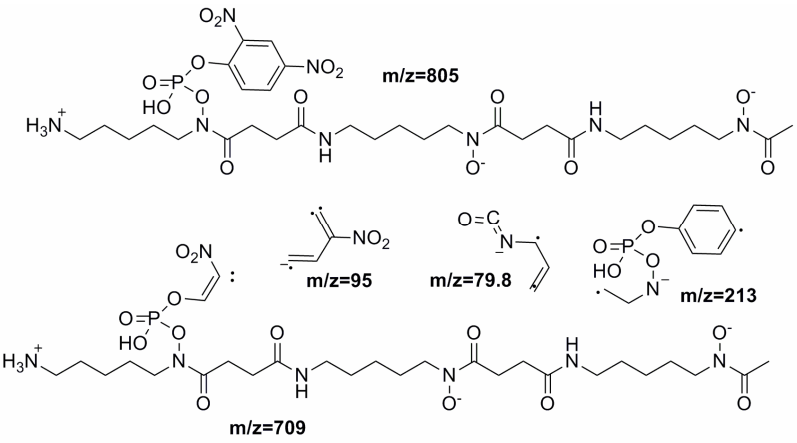
a. m/z fragments for **BDNPP** of m/z 429



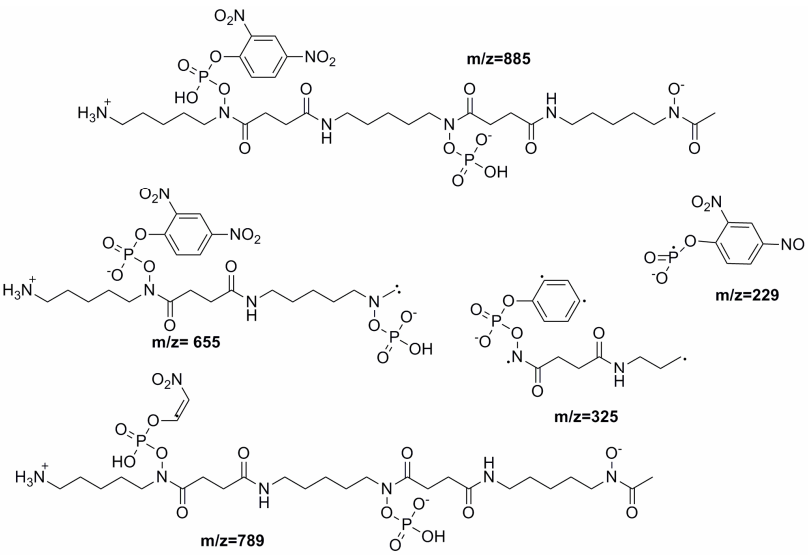
b. m/z fragments for **DFO** of m/z 559



c. m/z fragments for m/z 805



d. m/z fragments for m/z 885



The reactant **BDNPP** of m/z 429 dissociates to the fragments of m/z 245, 215, 183, 153, 137, 123, 109, 94.9 and 78.8 (**Figure S4, Scheme S3**), which are mainly due to loses of the nitro groups and ring opening reactions. Furthermore, **DFO** of m/z 559 dissociates to the fragments of m/z 441, 317, 259, 241, 199, 161, 155, 136, 97.9 and 58.9 (**Figure S5, Scheme S3**) and the fragments are consistent with multiple cleavages of the **DFO** anion, consistent with its complex and relatively large structure. The ESI-MS/MS of **BDNPP** and **DFO** were helpful in providing information about the nature of the phosphorylated intermediates.

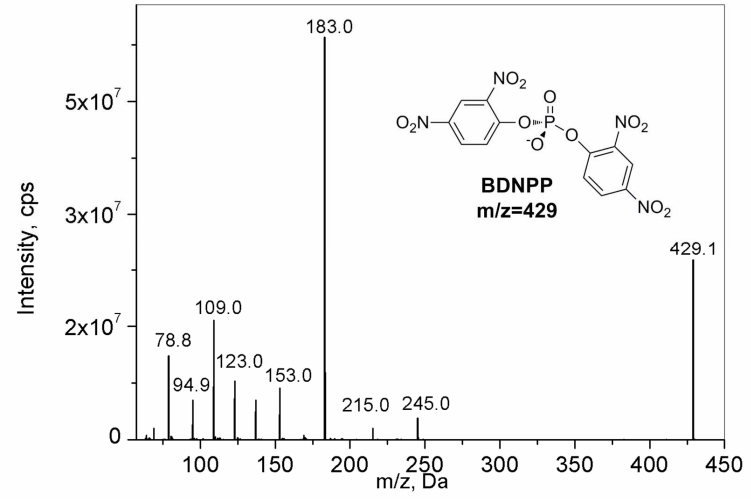


Figure S4. ESI-MS/MS of the reagent **BDNPP** of m/z 429.

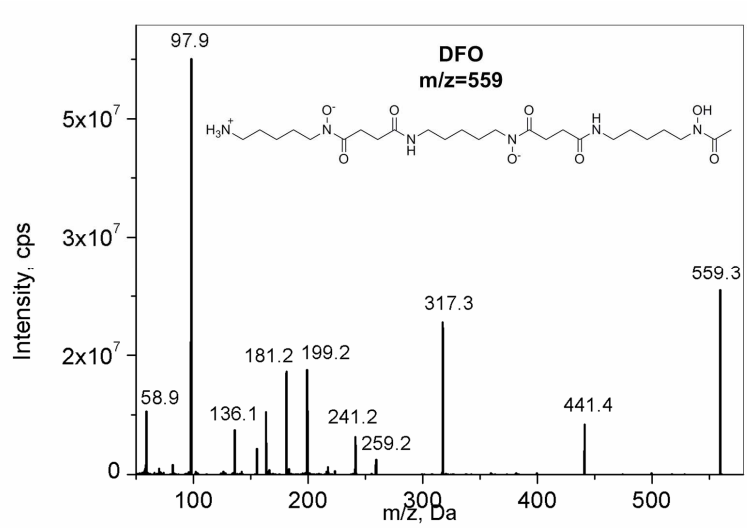


Figure S5. ESI-MS/MS of the reagent **DFO** of m/z 559.